

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.16e-10 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.72e-01

Confidence level: 3.13e-01

Nearest Neighbors from the Training Set

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9,10-Anthracenedione, 1,4-bis(methylamino)-  
**Measured:** 1.80e-08  
**Predicted:** 4.57e-11

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2,4,6-Trimethylpyridine  
**Measured:** 3.59e-10  
**Predicted:** 8.58e-01

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Cloxyfonac [ISO]  
**Measured:** 6.86e-12  
**Predicted:** 3.84e-07

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Lepidine  
**Measured:** 8.02e-14  
**Predicted:** 9.90e-03